LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG053019\
Data File : BG040957.D
Acq On : 30 May 2019 19:33
Operator : HP/JU
Sample : K3075-03
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TEST-PIT-2

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG052919.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.131	3	7	15	rVB2	114235	224184	4.43%	0.756%
2	3.208	15	20	34	rVB	424053	676933	13.37%	2.282%
3	5.658	429	437	448	rBV	1332630	2090100	41.29%	7.047%
4	7.268	703	711	722	rBV	1395711	2401109	47.43%	8.096%
5	7.650	768	776	785	rBV	1330134	2267663	44.79%	7.646%
6	8.120	849	856	868	rVB	224488	395990	7.82%	1.335%
7	8.449	903	912	919	rBV	943998	1642024	32.43%	5.536%
8	9.301	1047	1057	1067	rBV	842352	1479997	29.23%	4.990%
9	10.946	1330	1337	1346	rBV	284975	508913	10.05%	1.716%
10	13.378	1741	1751	1763	rBV	1960016	3090573	61.05%	10.420%
11	14.195	1884	1890	1896	rBV	307283	437009	8.63%	1.473%
12	14.753	1978	1985	1993	rBV2	473996	767592	15.16%	2.588%
13	16.240	2231	2238	2247	rBV	2102876	3114042	61.51%	10.500%
14	17.497	2443	2452	2463	rBV2	691329	1072480	21.18%	3.616%
15	18.349	2592	2597	2608	rBV2	364683	541759	10.70%	1.827%
16	19.612	2807	2812	2823	rBV2	98195	160609	3.17%	0.542%
17	20.094	2887	2894	2899	rBV	3863179	5062576	100.00%	17.069%
18	21.369	3106	3111	3124	rBV2	232127	422225	8.34%	1.424%
19	21.774	3173	3180	3190	rVB2	768200	1271126	25.11%	4.286%
20	21.927	3202	3206	3213	rVB2	45437	67096	1.33%	0.226%
21	22.550	3307	3312	3323	rVB3	62761	115949	2.29%	0.391%
22	23.261	3427	3433	3439	rBV	71623	126730	2.50%	0.427%
23	23.460	3460	3467	3475	rVB2	89670	188640	3.73%	0.636%
24	24.083	3567	3573	3582	rVB3	54566	130263	2.57%	0.439%
25	25.117	3735	3749	3764	rVB2	413920	1301316	25.70%	4.388%
26	26.245	3932	3941	3950	rVB7	32147	101730	2.01%	0.343%

Sum of corrected areas: 29658628

LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG053019\
Data File : BG040957.D
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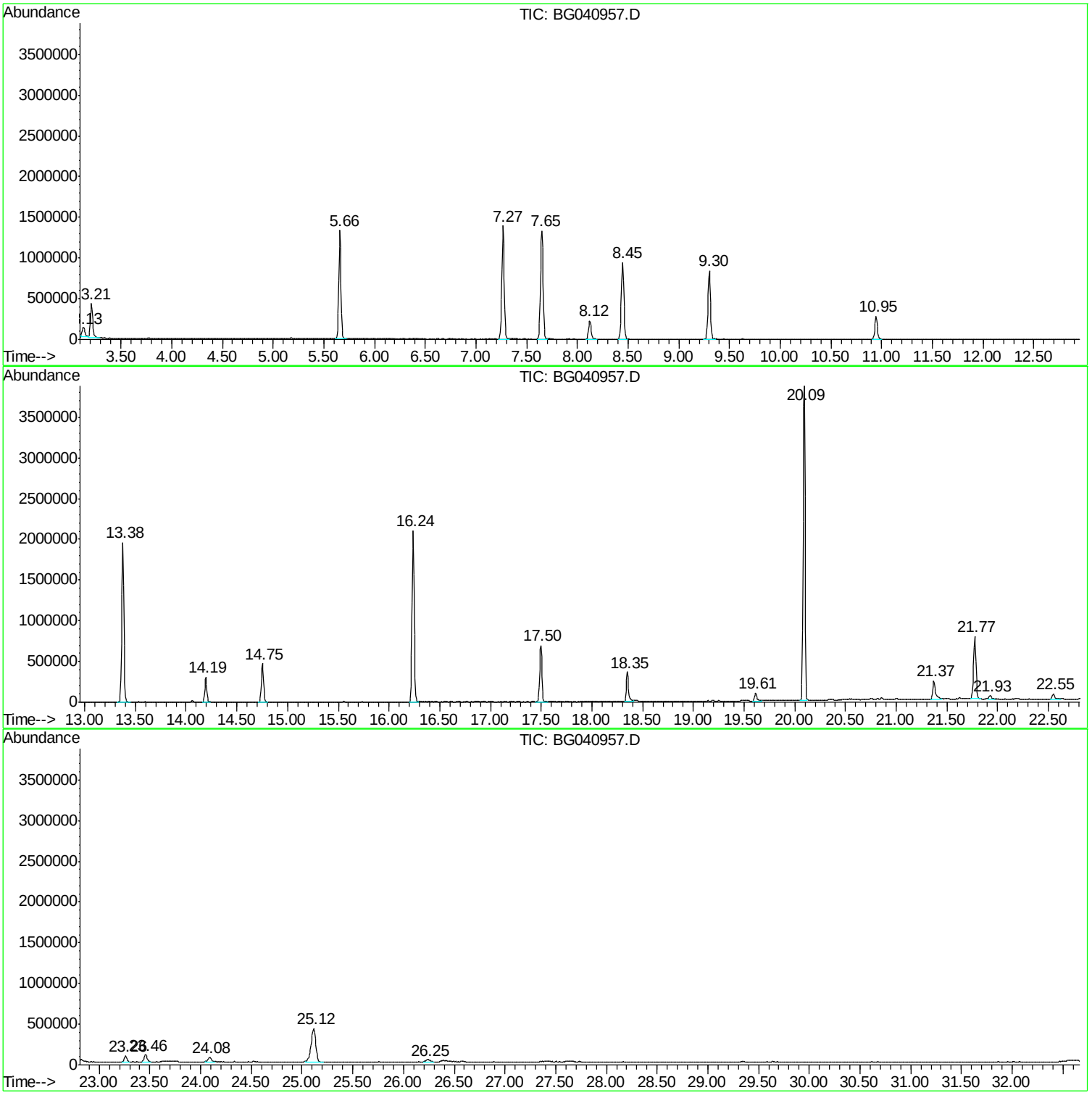
Operator : HP/JU
Sample : K3075-03
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TEST-PIT-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG052919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG053019\
Data File : BG040957.D
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Instrument : BNA_G
ClientSampleId : TEST-PIT-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG052919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

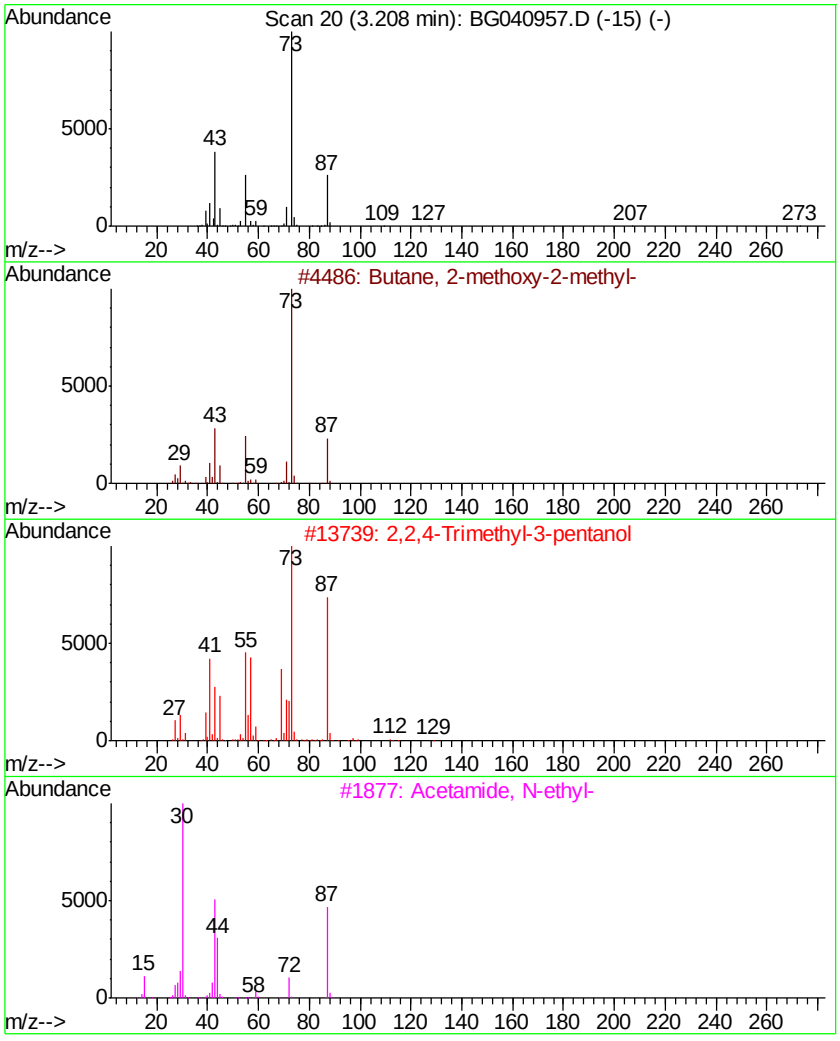
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

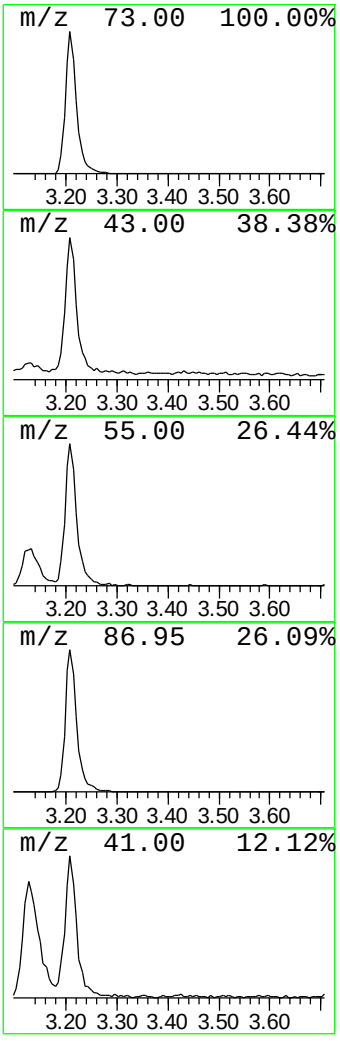
****

Peak Number 2 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.21	34.19 ng	676933	1,4-Dichlorobenzene-d4	8.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	27
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
5	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG053019\
Data File : BG040957.D
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Misc :
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Instrument : BNA_G
ClientSampleId : TEST-PIT-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG052919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

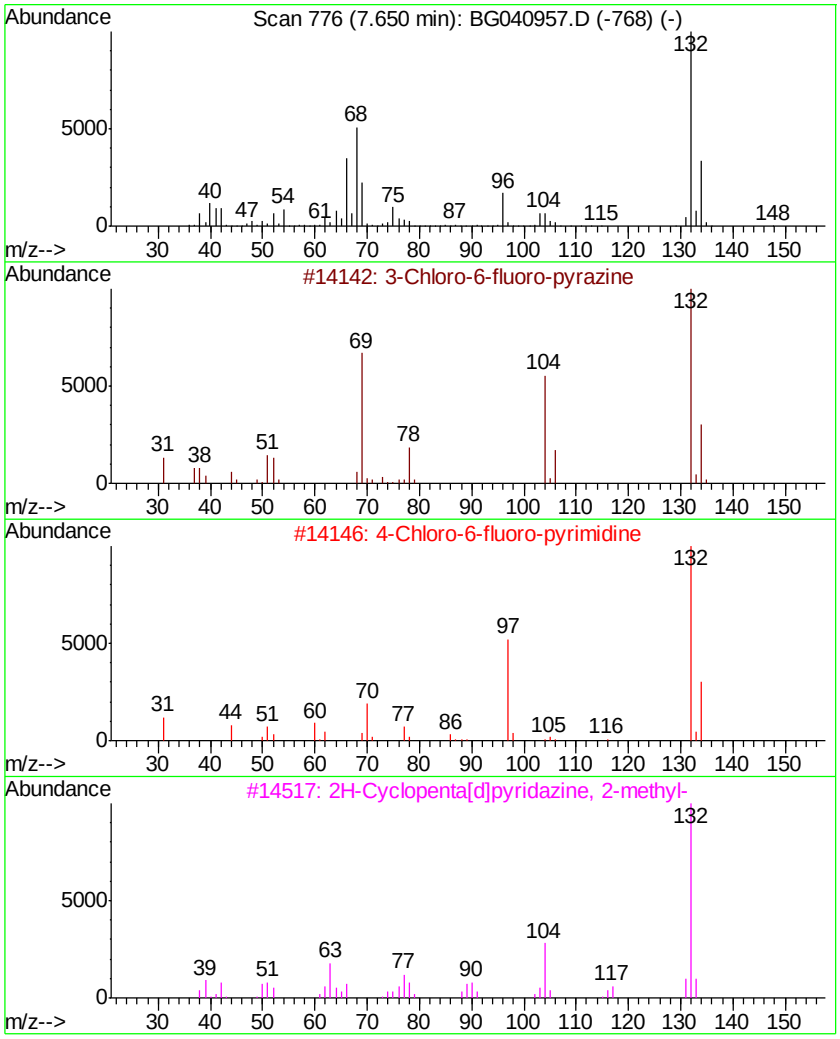
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

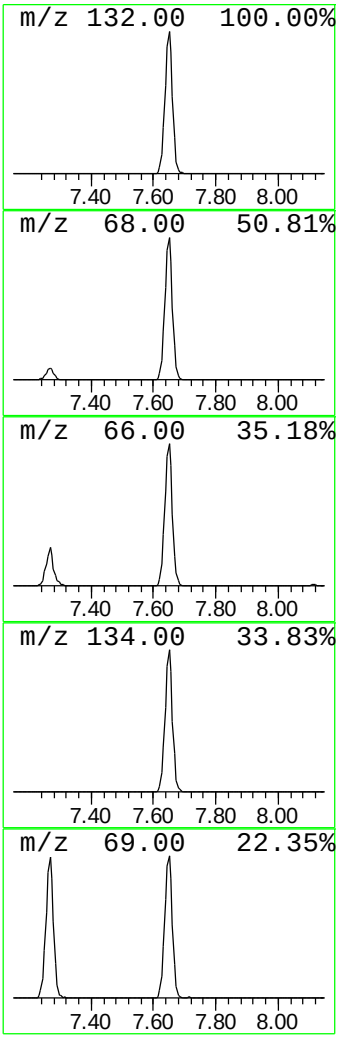
****

Peak Number 3 unknown7.65 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.65	114.53 ng	2267660	1,4-Dichlorobenzene-d4	8.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
3	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	22
4	Pyrazolo(2,3-a)pyridine, 7-methyl-	132	C8H8N2	034760-58-2	22
5	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	22





Library Search Compound Report

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Data File : BG040957.D
Acq On : 30 May 2019 19:33
Operator : HP/JU
Sample : K3075-03
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TEST-PIT-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG052919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

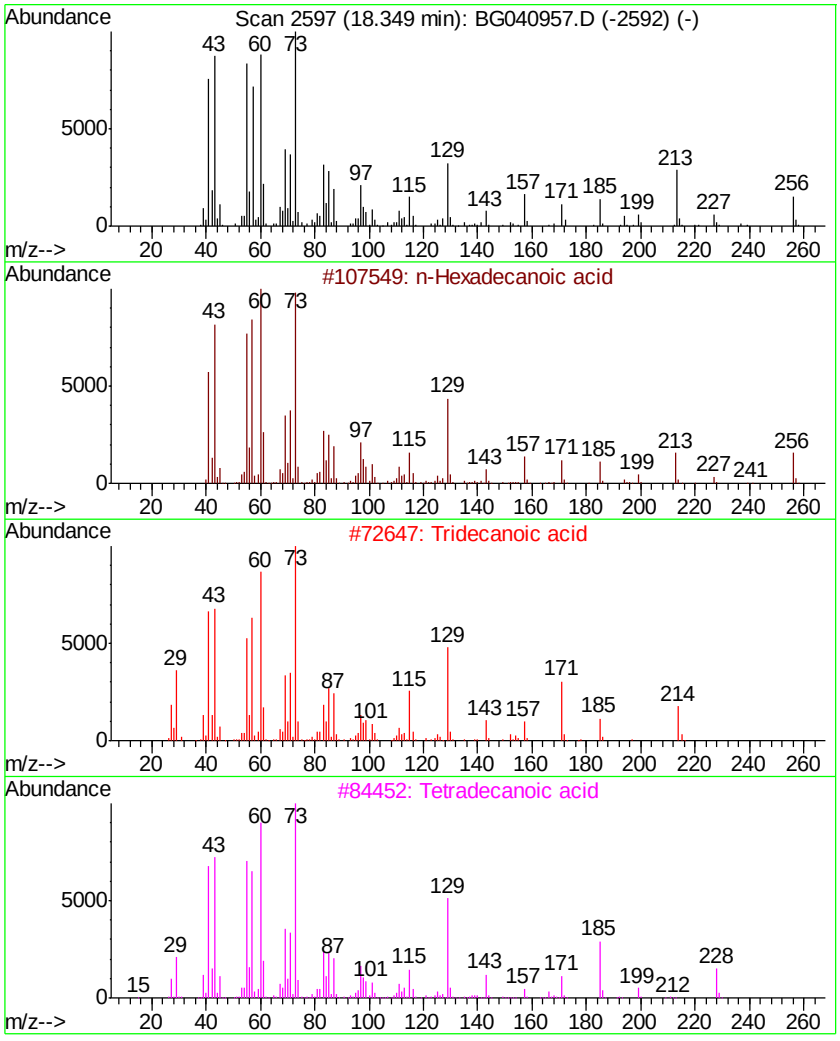
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

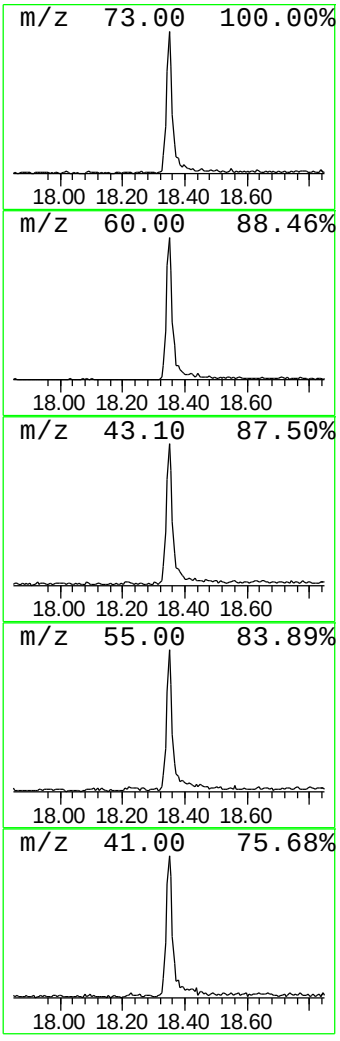
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.35	10.10 ng	541759	Phenanthrene-d10	17.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tridecanoic acid	214	C13H26O2	000638-53-9	95
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	93
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	76
5	n-Decanoic acid	172	C10H20O2	000334-48-5	53





Library Search Compound Report

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Data File : BG040957.D
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Operator : HP/JU
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Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TEST-PIT-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG052919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

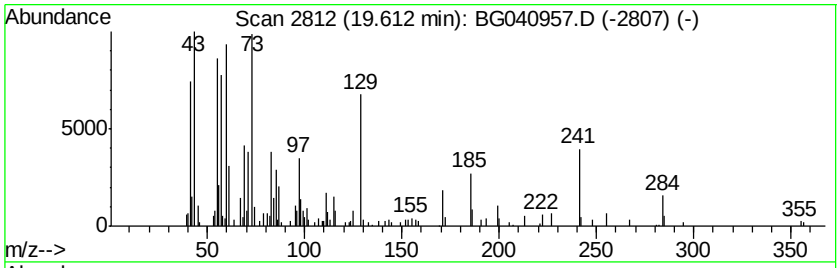
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

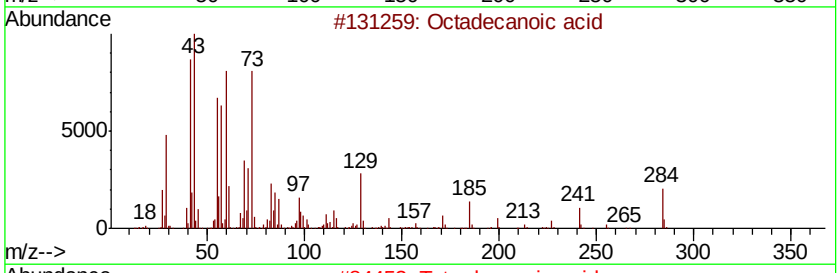
****

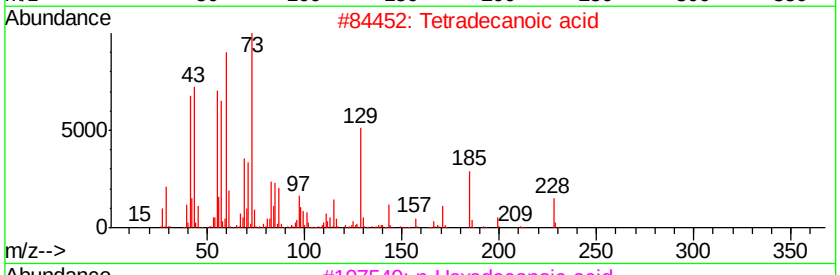
Peak Number 6 Octadecanoic acid Concentration Rank 7

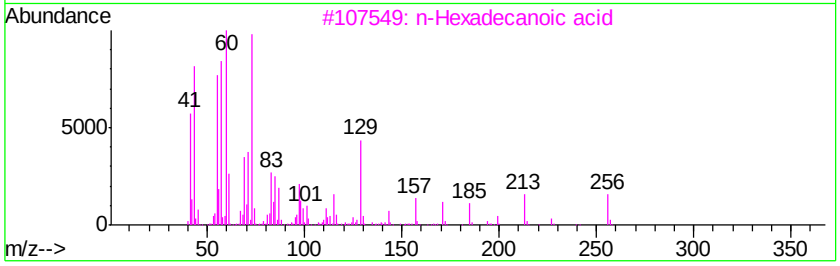
R.T.	EstConc	Area	Relative to ISTD	R.T.
19.61	3.00 ng	160609	Phenanthrene-d10	17.50

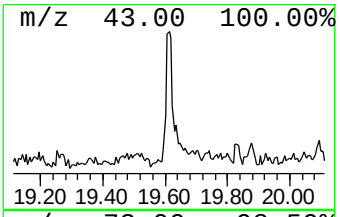
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	95
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	64
4	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	59
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	58

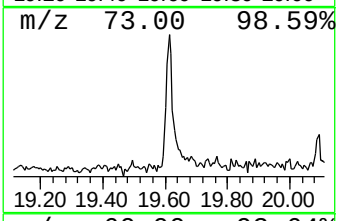


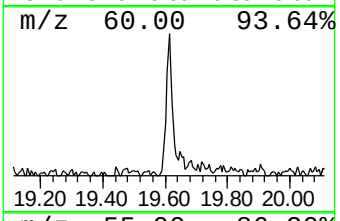


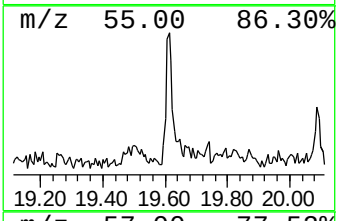


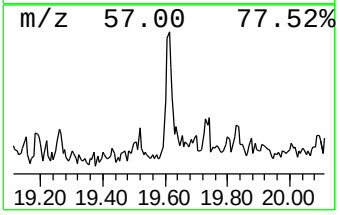












Library Search Compound Report

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Instrument : BNA_G
ClientSampleId : TEST-PIT-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG052919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

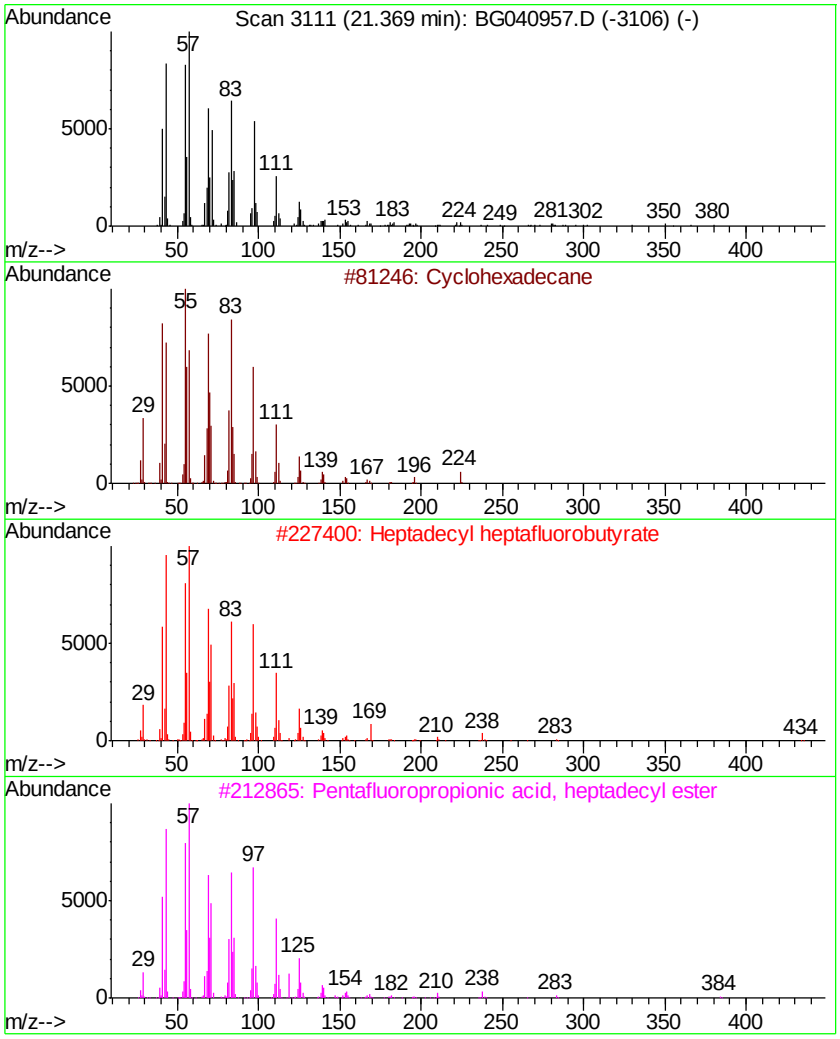
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

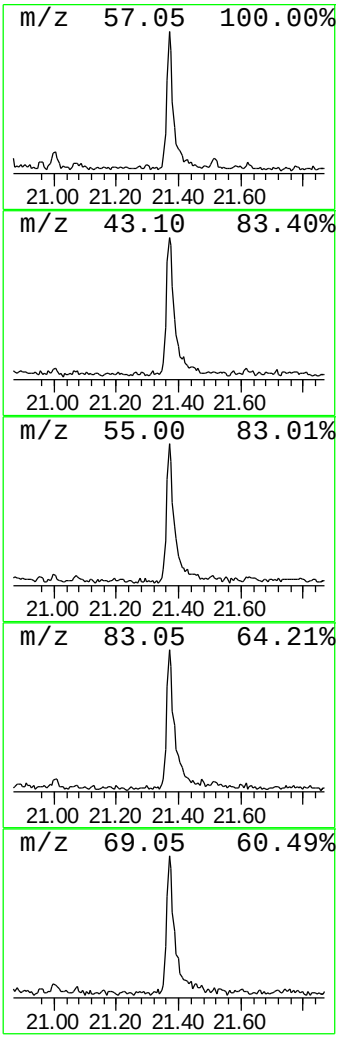
****

Peak Number 7 Cyclohexadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.37	6.64 ng	422225	Chrysene-d12	21.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexadecane	224	C16H32	000295-65-8	92
2	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	91
3	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	91
4	Nonadecyl trifluoroacetate	380	C21H39F3O2	1000351-76-3	91
5	Pentafluoropropionic acid, octad...	416	C21H37F5O2	959261-25-7	91





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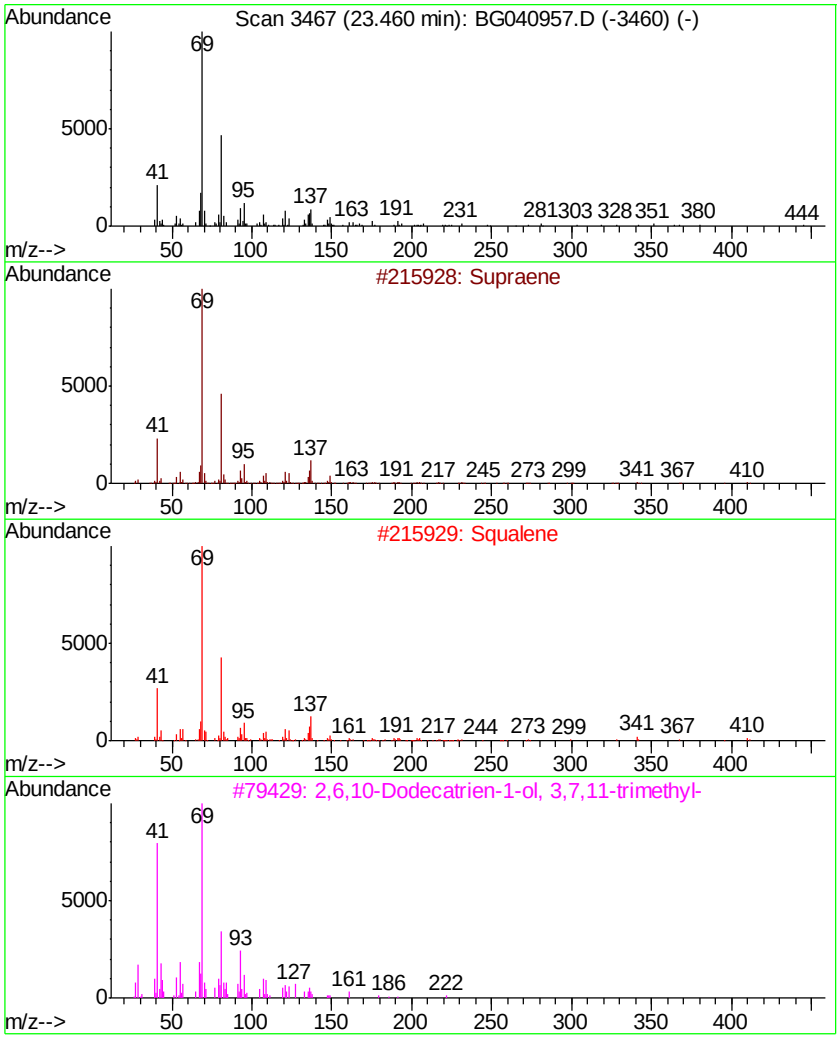
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

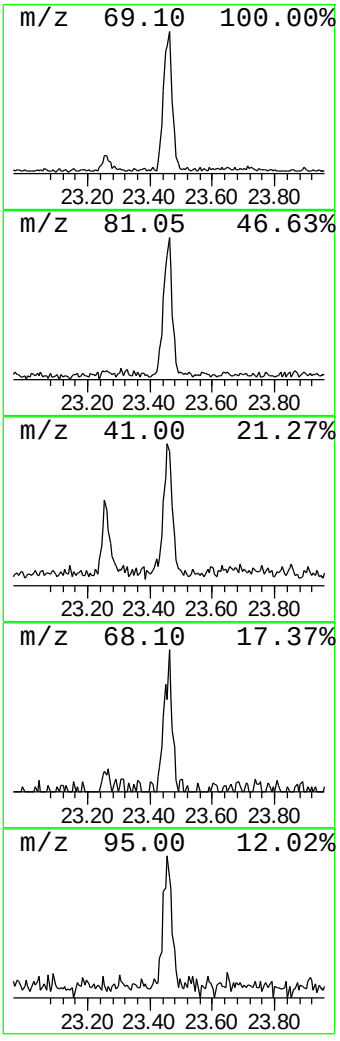
****

Peak Number 8 Supraene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.46	2.90 ng	188640	Perylene-d12	25.12

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Supraene	410	C30H50	007683-64-9	86
2	Squalene	410	C30H50	000111-02-4	72
3	2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	004602-84-0	64
4	.psi.,.psi.-Carotene, 7,7',8,8',...	547	C40H66	000502-62-5	64
5	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	64





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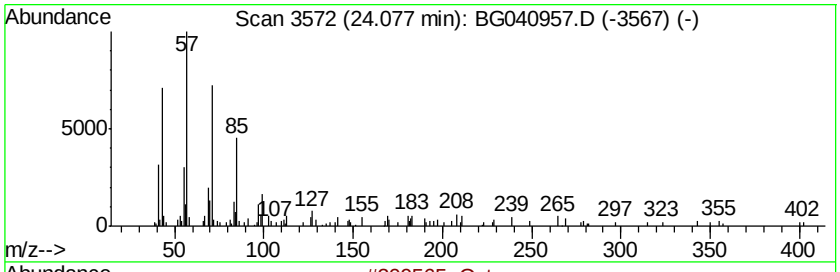
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

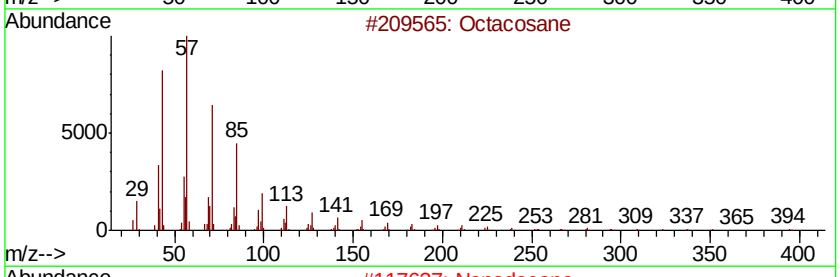
****

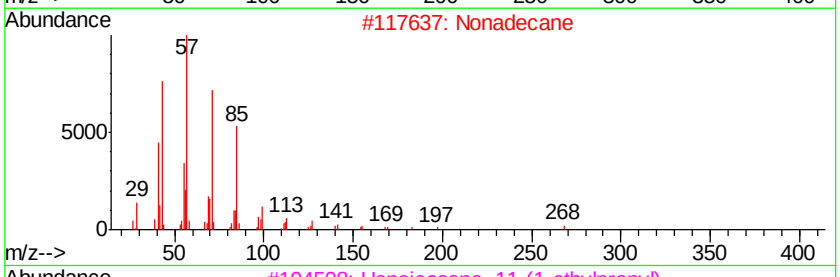
Peak Number 9 Octacosane Concentration Rank 9

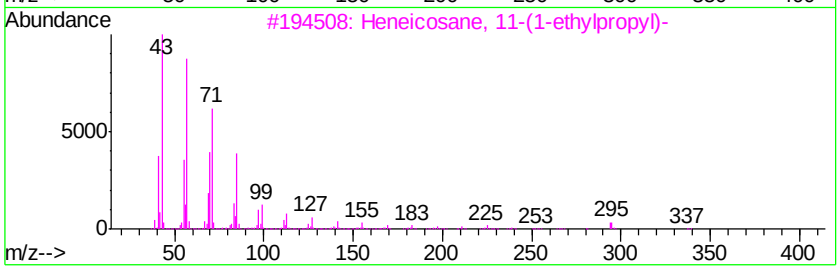
R.T.	EstConc	Area	Relative to ISTD	R.T.
24.08	2.00 ng	130263	Perylene-d12	25.12

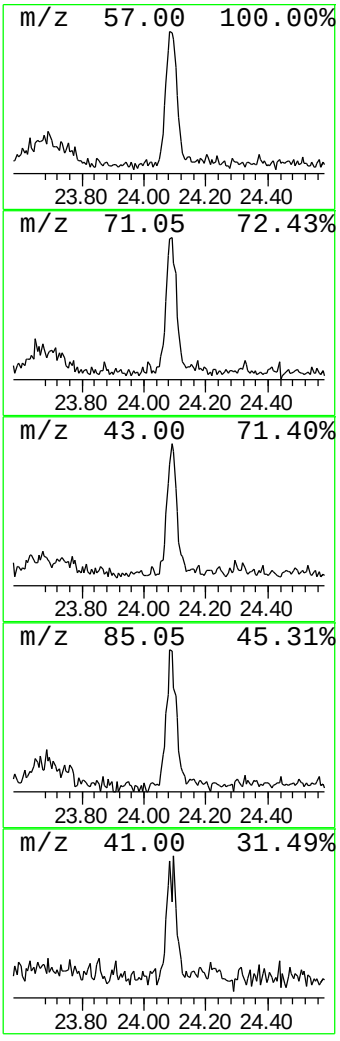
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	91
2	Nonadecane	268	C19H40	000629-92-5	90
3	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	90
4	Tetracosane	338	C24H50	000646-31-1	87
5	Triacontane	422	C30H62	000638-68-6	86











Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG053019\
Data File : BG040957.D
Acq On : 30 May 2019 19:33
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Misc :
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Instrument : BNA_G
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-methoxy...	3.21	34.2	ng	676933	1	8.13	395990	20.0
unknown7.65	7.65	114.5	ng	2267660	1	8.13	395990	20.0
n-Hexadecanoic acid	18.35	10.1	ng	541759	4	17.50	1072480	20.0
Octadecanoic acid	19.61	3.0	ng	160609	4	17.50	1072480	20.0
Cyclohexadecane	21.37	6.6	ng	422225	5	21.77	1271130	20.0
Supraene	23.46	2.9	ng	188640	6	25.12	1301320	20.0
Octacosane	24.08	2.0	ng	130263	6	25.12	1301320	20.0